Parallelization – when a single thread is not enough

Valentin Haenel
Strongly based on materials by Eilif Muller and Bastian Venthur

Freelance Consultant and Software Developer
http://haenel.co

Feb 2013

Version: 2013-02-pcp13.1-1-gd423122 https://git.example.com/example

Outline

Outline

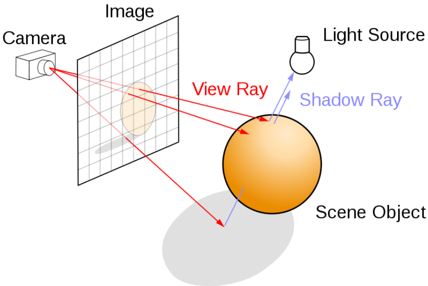
What is concurrency

- Parallel computing/processing
- Several computations executing simultaneously
- ... potentially interacting with each other

The brain is a parallel machine

- Asynchronous
- Distributed memory
- Simple messages
- Agnostic to component failure
- Connectivity:
  - dense local
  - sparse global
- Works with long latencies

Outline



Trace the path from an imaginary eye (camera) through each pixel in a screen and calculate the color of the object(s) visible through it.

Useful Applications for Concurrency

Ray Tracing

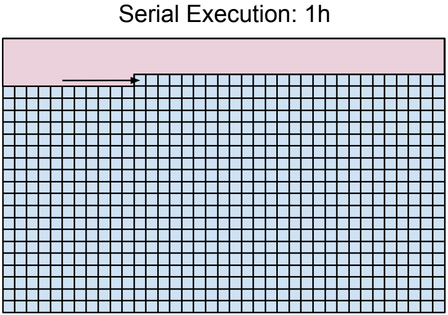


Figure: Ray Tracing performed by one task.

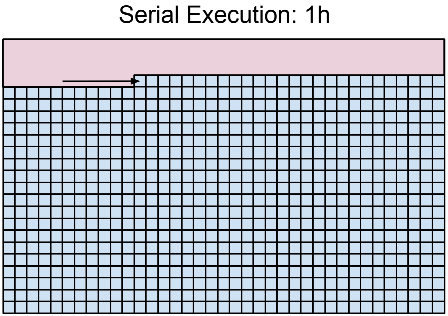


Figure: Ray Tracing performed by one task.

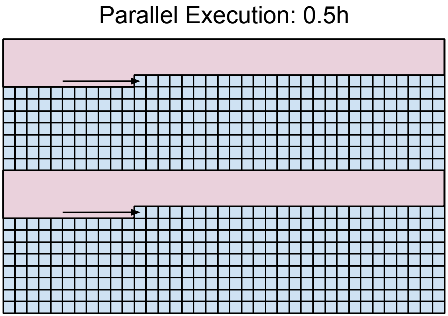


Figure: Ray Tracing performed by two tasks.

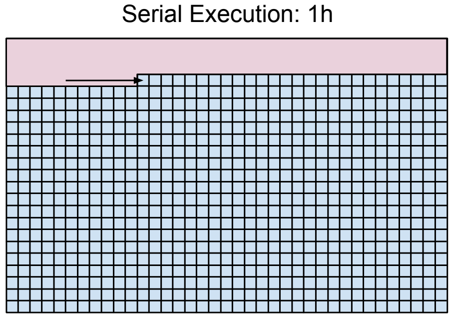


Figure: Ray Tracing performed by one task.

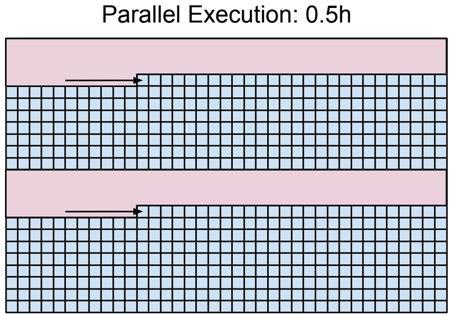


Figure: Ray Tracing performed by two tasks.

Ray Tracing is **embarrassingly parallel**:

- Little or no effort to separate the problem into parallel tasks
- No dependencies or communication between the tasks

Outline

The free lunch is over

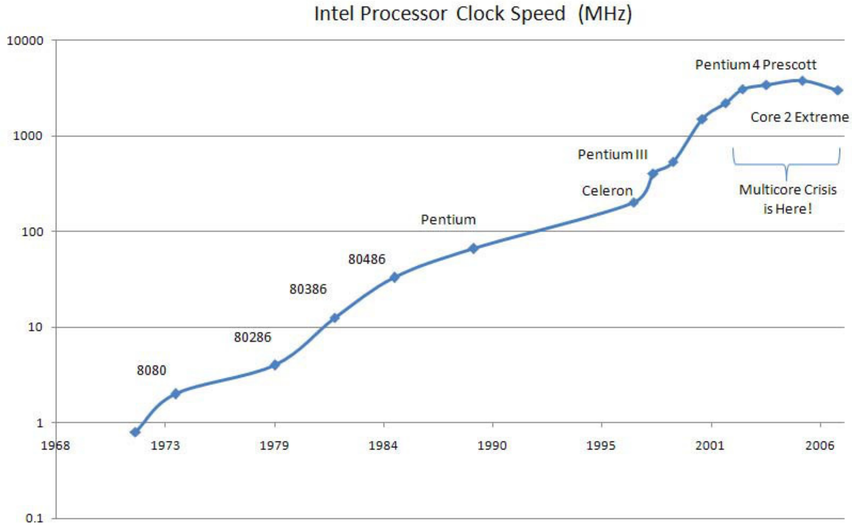
"Concurrency is the next major revolution in how we write software [after OOP]."

Herb Sutter, *The Free Lunch is Over: A Fundamental Turn Towards Concurrency in Software* Dr.Dobb's Journal, 30(3) March 2005.

Multicore Crisis

- 1970-2005
  - CPUs became quicker and quicker every year
  - Moore's Law: The number of transistors [...] doubles
  - approximately every two years.
- But!
  - Physical limits:
    - Miniaturization at atomic levels
    - energy consumption
    - heat produced by CPUs, etc.
  - Stagnation in CPU clock rates since 2005
- Since 2005
  - Chip producers aimed for more cores instead of higher clock rates.
  - $\Rightarrow$ Multicore crisis
  - FLOPS/S has been raplaced by FLOPS/W
  - (esp. in High Performance Computing(HPC))

Multicore Crisis



Don't Panic

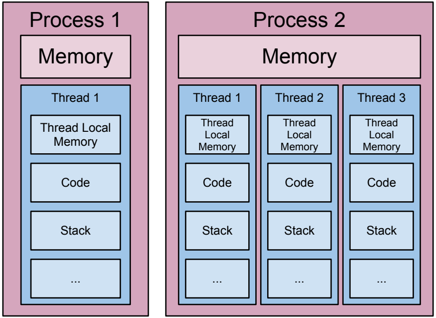
- Writing parallel programs is easy!
- Small and simple APIs
- Designing parallel algorithms can be easy or hard
- Easy: embarassingly parallel
- Hard: to find the parallelism

Don't Panic

- Scientific parallel programs are easy!
- Parallelism: Number crunching over large datasets
- Prior-art: Many algorithms already exist
- Hardware: HPC is traditionally academic

Outline

Two Kinds of Tasks: Threads and Processes



- A process has **one or more** threads
- Processes have their **own** memory (Variables, etc.)
- Threads share the memory of the process they belong to
- Threads are also called **lightweight** processes:
  - They spawn faster than processes
  - Context switches (if necessary) are faster

Basically you have two paradigms:

1. Shared Memory
    - Taks A and B share some memory
    - Whenever a task modifies a variable in the shared memory, the other task(s) see that change immediately
2. Message Passing
    - Task A sends a message to Task B
    - Task B receives the message and does something with it

The former paradigm is usually used with threads and the latter one with processes (more on that later).

Symmetric Multiprocessing (SMP)

- Homogeneous Multi-core and/or cpu
- Physically shared memory
- e.g. 8-way 6-core Opteron = 48 cores
- Most of you will have such a Laptop by now

Python and the Global Interpreter Lock

- Python suffers from the *Gil Problem*
- The interpreter has a global state storage
- Not thread-safe!

- Can have threads
- ... but only one can run at a time
- No real, concurrent threads in Python

SMP in Python

- Standard as of Python 2.6

```
>>> import multiprocessing
```

- Like threads, but in separate processes
- Avoids GIL but higher process creation cost
- Package exists for 2.5

Race

- When unpredictable order of completion affects output
  - Hardware latency
  - Unpredictable algorithm run-time
- Difficult to debug because problematic case maybe infrequent

Race: the setup

```
import multiprocessing as mp
import time
import random

def mult(arg):
    time.sleep(random.uniform(1,5))
    arg.value *= 10

def add(arg):
    time.sleep(random.uniform(1,5))
    arg.value += 10

arg = mp.Value('d', 0.0)  # synchronized shared object, type double

p1 = mp.Process(target=mult, args=(arg,))
p2 = mp.Process(target=add, args=(arg,))
p1.start(); p2.start(); p1.join(); p2.join()
print arg.value
```

Race: in action

```
$ python ex_smp_race.py
10.0
$ python ex_smp_race.py
100.0
$ python ex_smp_race.py
10.0
```

The apparent solution

- Locks can be a solution to enforce atomicity:

```
l = Lock()
l.acquire()
# <code>
l.release()
```

- However, Locks are source of deadlocks

Deadlock: the setup

```
import multiprocessing as mp

def compute(arg, lock):
    lock.acquire()
    arg.value += 10

arg = mp.Value('d', 0.0)  # synchronized shared object, type double
lock = mp.Lock()          # non-recursive lock object

p1 = mp.Process(target=compute, args=(arg, lock))
p2 = mp.Process(target=compute, args=(arg, lock))
p1.start()
p2.start()
p1.join()
```

Deadlock: in action

```
>>> %run ex_smp.py
# p2 is still waiting for release (deadlock)
>>> p2.is_alive()
True
>>> arg.value()
10.0
# resolve the deadlock, without killing processes
>>> lock.release()
>>> p2.is_alive()
False
>>> p2.join()
>>> num.value
20
```

See also: Dining Philosophers

Shared Memory: Numpy and Multiprocessing

```
import ctypes
from multiprocessing import sharedctypes, Process
import numpy
from numpy import ctypeslib

def f(cta):
    from numpy import ctypeslib
    npa = ctypeslib.as_array(cta._obj)
    npa[0] = npa.sum()

cta = sharedctypes.Array(ctypes.c_double, numpy.arange(1e6))
npa = ctypeslib.as_array(cta._obj)
p1 = Process(target=f, args=(cta,))
```

- cta is a synchronized shared memory buffer
- npa is a numpy array that shares memory with cta

Shared Memory: Numpy and Multiprocessing

```
>>> %run ex_smp_numpy.py
>>> npa
array([  0.00000000e+00,   1.00000000e+00,   2.00000000e+00, ...,
         9.99997000e+05,   9.99998000e+05,   9.99999000e+05])
>>> p1.start(); p1.join()
In [6]: npa
array([  4.99999500e+11,   1.00000000e+00,   2.00000000e+00, ...,
         9.99997000e+05,   9.99998000e+05,   9.99999000e+05])
```

Embarrassingly Parallel - Multiprocessing

- Imagine the following function that does work

```
def f(x):
    import time
    import random
    time.sleep(random.uniform(0.1, 0.2))
    return x*x

nums = range(10)
```

The `Pool` class and `map` function

- Python provides a builtin `map` function
- The `Pool` class comes in handy for embarrassingly parallel problems
- Provides a `map` function across worker processes

```
>>> nums = range(10)
>>> %timeit map(f, nums)
1 loops, best of 3: 1.52 s per loop
>>> pool1 = Pool(1)
>>> %timeit pool1.map(f, nums)
1 loops, best of 3: 1.32 s per loop
>>> pool6 = Pool(6)
>>> %timeit pool6.map(f, nums)
1 loops, best of 3: 327 ms per loop
>>> pool24 = Pool(24)
>>> %timeit pool24.map(f, nums)
10 loops, best of 3: 187 ms per loop
```

- `import` statements need to be in the function
- If you need one with a progressbar: embparpbar

Outline

Starting IPython engines

- To launch a small (or large) cluster of IPython engines

```
$ ipcluster start -n 24
2013-02-05 16:35:56,367.367 [IPClusterStart]
    Using existing profile dir: u'/home/val/.ipython/profile_default'
2013-02-05 16:35:56.372 [IPClusterStart]
    Starting ipcluster with [daemon=False]
2013-02-05 16:35:56.373 [IPClusterStart]
    Creating pid file: /home/val/.ipython/profile_default/pid/ipcluster.p
2013-02-05 16:35:56.376 [IPClusterStart]
    Starting Controller with LocalControllerLauncher
2013-02-05 16:35:57.372 [IPClusterStart]
    Starting 24 Engines with LocalEngineSetLauncher
2013-02-05 16:36:29.888 [IPClusterStart]
    Engines appear to have started successfully
```

Command them from IPython

- Use the `Client` class to interface with the engines

```
>>> from IPython.parallel import Client
>>> client = Client()
>>> len(client.ids)
24
```

- Easy example: using an embarrassingly parallel map
- Obtain a `DirectView` using slicing on the `client`

```
>>> dview = client[:]
>>> type(dview)
IPython.parallel.client.view.DirectView
>>> %timeit dview.map_sync(f, range(10)) # using the f from before
1 loops, best of 3: 187 ms per loop
```

IPython engines have local namespaces

- `DirectView` object provides dictionary access to engine namespaces

```
>>> dview.execute('x=1')
>>> dview['x']
[1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1]
>>> dview8 = client[8]
>>> dview8.execute('x=23')
>>> dview['x']
[1, 1, 1, 1, 1, 1, 1, 1, 23, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1]
```

- Using `apply` in asynchronous and synchronous mode

```
>>> result = dview.apply(lambda y: x+y, 19)
>>> type(result)
IPython.parallel.client.asyncresult.AsyncResult
>>> result.get()[7:12]
[20, 42, 20, 20, 20]
>>> dview.block = True
>>> dview.apply(lambda y: x+y, 19)
...
```

Partition and Collection data

- Send using `scatter`

```
>>> dview4 = client[:4]
>>> dview4.block = True
>>> dview4.scatter('a','Hello World!')
['Hel', 'lo ', 'Wor', 'ld!']
```

- Now operate on the data using `execute`

```
>>> dview4.execute('a = a.upper()', targets=[0, 1])
>>> dview4['a']
['HEL', 'LO ', 'Wor', 'ld!']
```

- Collect using `gather`

```
>>> "".join(dview4.gather('a'))
'HELLO World!'
```

Warnings

- Engines are not reset after IPython restart

```
>>> from IPython.parallel import Client
>>> client = Client()
>>> dview4 = client[:4]
>>> dview4['a']
['HEL', 'LO ', 'Wor', 'ld!']
```

- Errors propagate as usual

```
>>> dview8['b']
---------------------------------------------------------------------------
NameError                                 Traceback (most recent call last)
/home/val/anaconda/lib/python2.7/site-packages/IPython/parallel/util.py in
    249     else:
    250         if not user_ns.has_key(keys):
--> 251             raise NameError("name '%s' is not defined"%keys)
    252         return user_ns.get(keys)
    253
NameError: name 'b' is not defined
```

Pros and Cons

Pros

- Interactive
- Plays nicely with MPI
- Re-conectible
- Debugging output from engines
- Can be run over other batch queueing systems
  - (e.g. Sun Grid Engine)

Cons

- Slow for large messages
- No shared memory

Outline

Scalable Message Passing Concurrency

- MPI - the Message Passing Interface
- Multi-process execution facilities

```
$ mpiexec -n 16 python helloworld.py
```

- API for inter-process message exchanges
  - eg. Basic P2P: Send (emitter), Recv (consumer)
- Very common on large HPC installations

What is MPI for Python? (`mpi4py`)

- A wrapper for widely used MPI (MPICH2, OpenMPI, LAM/MPI)
- MPI supported by wide range of vendors, hardware, languages
- API based on the standard MPI-2 C++ bindings.
- Almost all MPI calls are supported.
  - targeted to MPI-2 implementations.
  - also works with MPI-1 implementations.

Basic stuff

```
from mpi4py import MPI
comm = MPI.COMM_WORLD
```

- Communicator = `comm`
  - Manages processes and communication between them
- `MPI.COMM_WORLD`
  - all processes defined at execution time
- `Comm.size` – total number of available processes
- `Comm.rank` – ID of the current process

Basic stuff

```python
from mpi4py import MPI
comm = MPI.COMM_WORLD
print "Hello from %s, %d of %d"\
    % (MPI.Get_processor_name(),
    comm.rank, comm.size)
```

```
$ mpiexec -n 4 python test.py
Hello from teik, 1 of 4
Hello from teik, 3 of 4
Hello from teik, 2 of 4
Hello from teik, 0 of 4
```

- Process needs to check which `rank` it is

What can this look like in practice

```
Hello, World! I am process 232 of 512 on Rank 232 of 512 <2,2,3,0>  R00-M0-N09-J18.
Hello, World! I am process 133 of 512 on Rank 133 of 512 <1,0,2,1>  R00-M0-N09-J04.
Hello, World! I am process 208 of 512 on Rank 208 of 512 <0,1,3,0>  R00-M0-N09-J26.
Hello, World! I am process 145 of 512 on Rank 145 of 512 <0,1,2,1>  R00-M0-N09-J22.
Hello, World! I am process 224 of 512 on Rank 224 of 512 <0,2,3,0>  R00-M0-N09-J25.
Hello, World! I am process 215 of 512 on Rank 215 of 512 <1,1,3,3>  R00-M0-N09-J09.
Hello, World! I am process 225 of 512 on Rank 225 of 512 <0,2,3,1>  R00-M0-N09-J25.
Hello, World! I am process 148 of 512 on Rank 148 of 512 <1,1,2,0>  R00-M0-N09-J05.
Hello, World! I am process 218 of 512 on Rank 218 of 512 <2,1,3,2>  R00-M0-N09-J17.
Hello, World! I am process 253 of 512 on Rank 253 of 512 <3,3,3,1>  R00-M0-N09-J32.
Hello, World! I am process 212 of 512 on Rank 212 of 512 <1,1,3,0>  R00-M0-N09-J09.
Hello, World! I am process 249 of 512 on Rank 249 of 512 <2,3,3,1>  R00-M0-N09-J19.
Hello, World! I am process 132 of 512 on Rank 132 of 512 <1,0,2,0>  R00-M0-N09-J04.
Hello, World! I am process 130 of 512 on Rank 130 of 512 <0,0,2,2>  R00-M0-N09-J23.
Hello, World! I am process 150 of 512 on Rank 150 of 512 <1,1,2,2>  R00-M0-N09-J05.
Hello, World! I am process 149 of 512 on Rank 149 of 512 <1,1,2,1>  R00-M0-N09-J05.
Hello, World! I am process 184 of 512 on Rank 184 of 512 <2,3,2,0>  R00-M0-N09-J15.
Hello, World! I am process 159 of 512 on Rank 159 of 512 <3,1,2,3>  R00-M0-N09-J30.
Hello, World! I am process 211 of 512 on Rank 211 of 512 <0,1,3,3>  R00-M0-N09-J26.
Hello, World! I am process 163 of 512 on Rank 163 of 512 <0,2,2,3>  R00-M0-N09-J21.
Hello, World! I am process 142 of 512 on Rank 142 of 512 <3,0,2,2>  R00-M0-N09-J31.
Hello, World! I am process 178 of 512 on Rank 178 of 512 <0,3,2,2>  R00-M0-N09-J20.
Hello, World! I am process 136 of 512 on Rank 136 of 512 <2,0,2,0>  R00-M0-N09-J12.
Hello, World! I am process 193 of 512 on Rank 193 of 512 <0,0,3,1>  R00-M0-N09-J27.
Hello, World! I am process 190 of 512 on Rank 190 of 512 <3,3,2,2>  R00-M0-N09-J28.
Hello, World! I am process 204 of 512 on Rank 204 of 512 <3,0,3,0>  R00-M0-N09-J35.
Hello, World! I am process 216 of 512 on Rank 216 of 512 <2,1,3,0>  R00-M0-N09-J17.
Hello, World! I am process 185 of 512 on Rank 185 of 512 <2,3,2,1>  R00-M0-N09-J15.
```

Point-to-Point (P2P): Python objects

```
from mpi4py import MPI

comm = MPI.COMM_WORLD
rank = comm.Get_rank()

if rank == 0:
    data = {'a': 7, 'b': 3.14}
    comm.send(data, dest=1, tag=11)
elif rank == 1:
    data = comm.recv(source=0, tag=11)
```

- The tag information allows selectivity of messages at the receiving end.

P2P: (NumPy) array data

```
from mpi4py import MPI
import numpy

comm = MPI.COMM_WORLD
rank = comm.Get_rank()

if rank == 0:
    data = numpy.arange(23, dtype='i')
    comm.Send([data, MPI.INT], dest=1, tag=77)
elif rank == 1:
    data = numpy.empty(23, dtype='i')
    comm.Recv([data, MPI.INT], source=0, tag=77)
```

- Array data buffer notation: [<BUFFER>, MPI.<DATATYPE>]
- Can also inferr the correct datatype from the numpy array
- MPI will write into the Numpy array

Collective Messages

Involve the whole `COMM`

- **Scatter**
  - Spread a sequence over processes
- **Gather**
  - Collect a sequence scattered over processes
- **Broadcast**
  - Send a message to all processes
- **Barrier**
  - Block till all processes arrive

Scatter and Gather

```python
from mpi4py import MPI
import numpy

comm = MPI.COMM_WORLD
rank = comm.Get_rank()

N = 10
# rank 0 should send the message
if comm.rank == 0:
    msg = numpy.arange(N, dtype=int)
else:
    msg = None

# dest should hold the scattered message
dest = numpy.empty(N/comm.size, dtype=int)
# ans should hold the gathered result
ans = numpy.empty(comm.size, dtype=int)
```

Scatter and Gather

```
# scatter the array
comm.Scatter([msg, MPI.INT],
             [dest, MPI.INT], root=0)

# do the work
mysum = numpy.sum(dest)

# gather the result
comm.Gather([mysum, MPI.INT],
            [ans, MPI.INT], root=0)
```

What is happening here

- Imagine `comm.size == 2`
- `len(dest)` is 5 everywhere
- `msg` is `array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])`
- `dest` on `0` becomes `array([0, 1, 2, 3, 4])`
- `dest` on `1` becomes `array([5, 6, 7, 8, 9])`

What is happening here

- Imagine `comm.size == 2`
- `len(dest)` is 5 everywhere
- `msg` is `array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])`
- `dest` on 0 becomes `array([0, 1, 2, 3, 4])`
- `dest` on 1 becomes `array([5, 6, 7, 8, 9])`
- What is the `len` of `ans`?

What is happening here

- Imagine `comm.size == 2`
- `len(dest)` is 5 everywhere
- `msg` is `array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])`
- `dest` on 0 becomes `array([0, 1, 2, 3, 4])`
- `dest` on 1 becomes `array([5, 6, 7, 8, 9])`

- What is the `len` of `ans`?
- 2 is correct

What is happening here

- Imagine `comm.size == 2`
- `len(dest)` is 5 everywhere
- `msg` is `array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])`
- `dest` on 0 becomes `array([0, 1, 2, 3, 4])`
- `dest` on 1 becomes `array([5, 6, 7, 8, 9])`

- What is the `len` of `ans`?
- 2 is correct
- What is the final value of `ans`?

What is happening here

- Imagine `comm.size == 2`
- `len(dest)` is 5 everywhere
- `msg` is `array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])`
- `dest` on 0 becomes `array([0, 1, 2, 3, 4])`
- `dest` on 1 becomes `array([5, 6, 7, 8, 9])`

- What is the `len` of `ans`?
- 2 is correct
- What is the final value of `ans`?
- `[10, 35]` is correct

The import problem

- Importing Python module from each MPI process may cause problems on big installations
- MPI_import provides specialised import statements that use MPI under the hood e.g. `mpi_import`

```
from MPI_Import import mpi_import, MPI
with mpi_import():
    import os
    import re
    import math
    import decimal
    import optparse
    import platform
    import string
    import zipfile
    import numpy

comm = MPI.COMM_WORLD
rank, size = comm.Get_rank(), comm.Get_size()
print "Hello World! I am rank %d of size %d"  % (rank, size)
```

Implementation

- Implemented with Cython
- Code base far easier to write, maintain, and extend.
- Faster than other solutions (mixed Python and C codes).
- A **pythonic** API that runs at C speed !

Portability

- Tested on all major platforms (Linux, Mac OS X, Windows).
- Works with the open-source MPI's (MPICH2, Open MPI, MPICH1, LAM).
- Should work with vendor-provided MPI's (HP, IBM, SGI).
- Works on Python 2.3 to 3.0 (Cython is just great!).

Interoperability

- Good support for wrapping other MPI-based codes.
- You can use Cython (`cimport` statement).
- You can use boost.
- You can use SWIG (*typemaps* provided).
- You can use F2Py (“py2f()“/“f2py()“ methods).
- You can use hand-written C (C-API provided).

- `mpi4py` will allow you to use virtually **any** MPI based C/C++/Fortran

code from Python.

Features Summary

- Classical MPI-1 Point-to-Point.
  - blocking (`send`/`recv`)
  - non-blocking (`isend`/`irecv`, `test`/`wait`).
- Classical MPI-1 and Extended MPI-2 Collectives.
- Communication of general Python objects (pickle).
  - very convenient, as general as pickle can be.
  - can be slow for large data (CPU and memory consuming).
- Communication of array data (Python's buffer interface).
  - MPI datatypes have to be explicitly specified.
  - Very fast, almost C speed (for messages above 5-10 kB).